Project 1 — Distributed Training on NYC Taxi (MPI)

Course: DSS5208 – Scalable Distributed Computing for Data Science
Goal: Train a 1-hidden-layer neural network on NYC taxi data using **MPI (mpi4py)**.
We run a σ×M sweep (activations × batch sizes), log training histories, report RMSE on train/test, and measure strong scaling (P = 1, 2, 4, 8).
Data are stored **nearly evenly** across processes via memory-mapped shards.

1) Data & Preprocessing

- **Raw:** `nytaxi2022.csv` (not tracked in Git).
- **Cleaned:** `nytaxi2022_cleaned.npz` created once with `data_prep.py`.
- **Even storage (memmap):** `prep_memmap_from_npz.py` exports:

```
memmap_data/
  X_train.npy, y_train.npy, X_test.npy, y_test.npy, meta.json
```

Each MPI rank mmaps only its slice of `[X_train, y_train]` and `[X_test, y_test]`.

Test RMSE is computed in parallel by slicing test shards per rank and reducing.

2) Model & Training

- **Network:** 1 hidden layer, linear output
  [\hat{y} = w_2^\top ,\sigma(W_1 x + b_1) + b_2]
- **Loss proxy logged each `eval_every`:** `R(θ_k)` = sampled MAE (fast to compute).
- **Optimizer:** plain SGD (mini-batches). Gradients averaged with `MPI.Allreduce`.
- **Key speed/robustness choices**
- memmap shards (**even storage & load**)
- `--eval_sample` for quick R(θk) and **`--eval_block`** for chunked RMSE (≈100k)
- **float32 no-copy** casts on load
- BLAS threads pinned: `OPENBLAS/MKL/NUMEXPR/OMP_NUM_THREADS=1` per MPI rank

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3) Experiment Grid (σ × M)

We swept **3 activations** × **5 batch sizes** at **P=4**. Hidden units **n** chosen per activation/M:

Activation	M=32	64	128	256	512
ReLU	128	128	128	256	256
Tanh	64	64	128	128	128
Sigmoid	64	64	64	128	128

Common settings: `lr=1e-3`, `epochs=1`, `seed=123`, `eval_every=1000`, `eval_sample=2e6`, `eval_block=100000`.

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4) Results (Sweep @ P=4)

Top-5 overall (from `results/top5_overall.csv`):

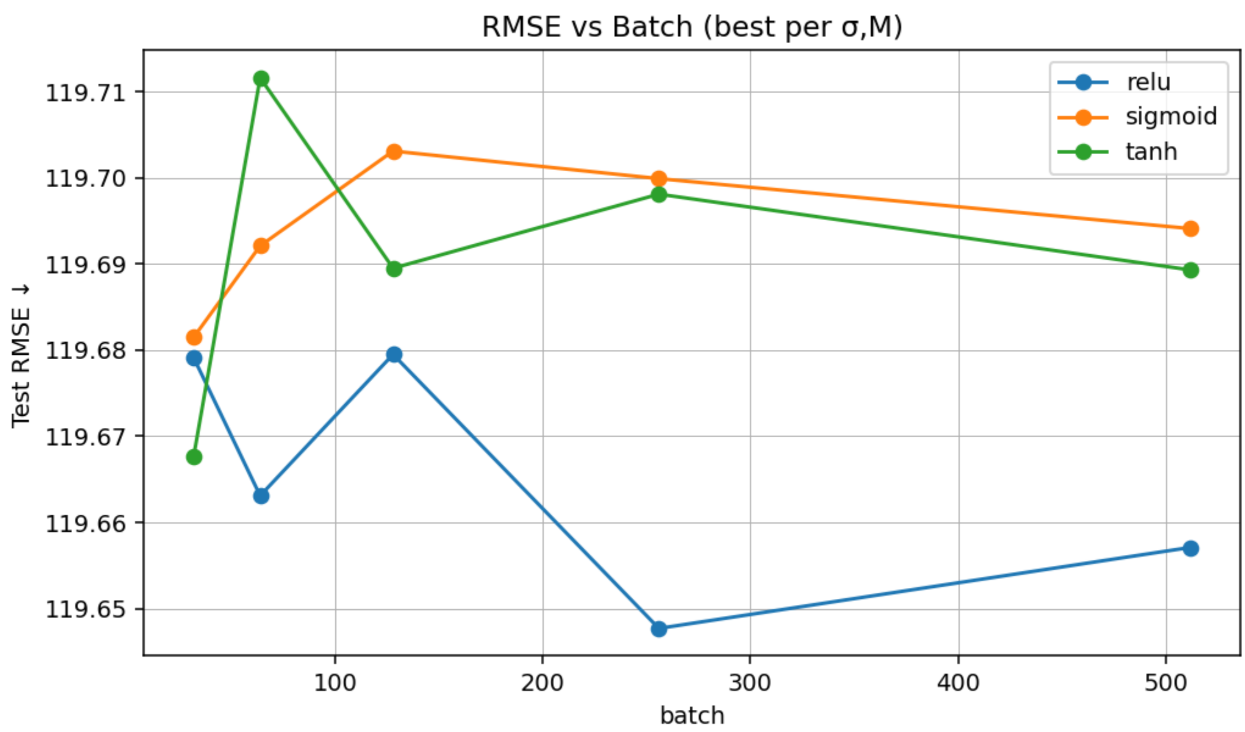
```
activation,batch,hidden,lr,procs,train_time,rmse_train,rmse_test
relu,512,256,0.001,4,177.863,85.8184,119.6571
relu,64,128,0.001,4,49.746,85.8283,119.6631
tanh,32,64,0.001,4,67.749,85.8356,119.6677
relu,256,256,0.001,4,60.513,85.8439,119.6749
relu,256,256,0.001,4,62.335,85.8439,119.6749
```

Observations

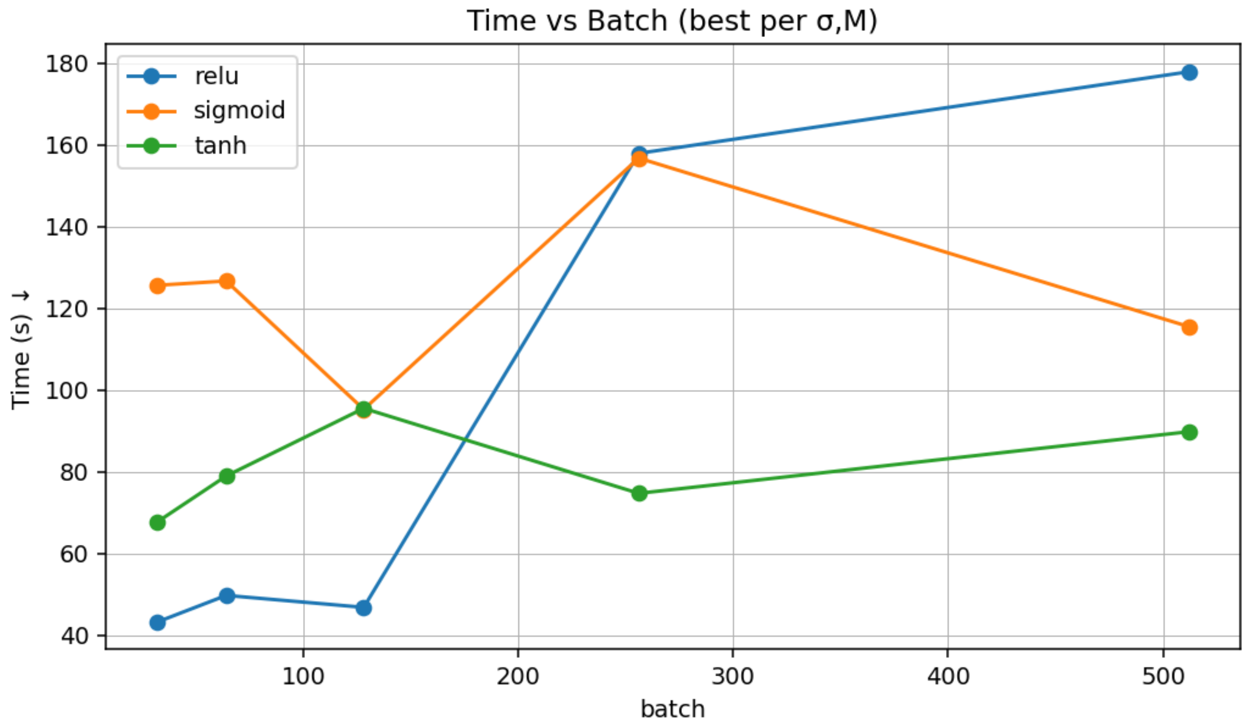
- RMSE is **stable** across σ and M (≈ 85.8 / 119.6).
- The **balanced** config `relu, M=256, n=256` gives competitive RMSE at good speed.
- Very large batch (`M=512`) is **slower** in wall-clock for 1 epoch on this CPU: larger matmuls per step + communication/compute balance.

Figures (produced by `summarize_results.py`):

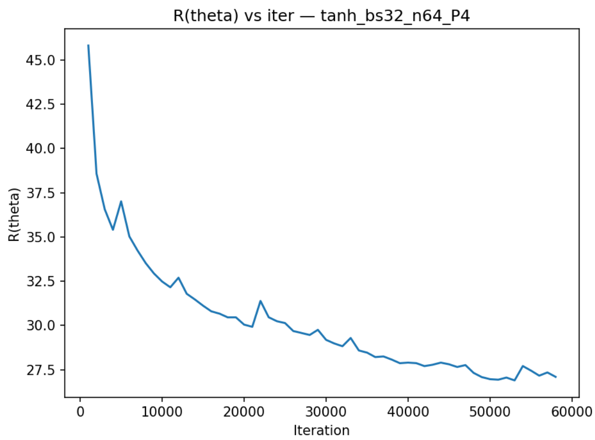
- **RMSE vs batch size**

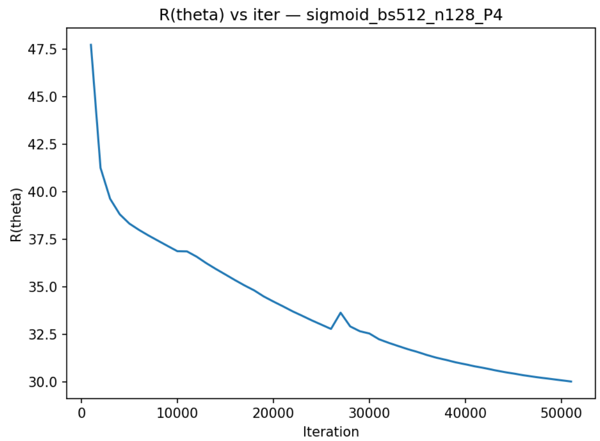


- **Training time vs batch size**



- **Sample training histories (P=4)**





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5) Strong Scaling (Fixed Config)

Config: `relu, M=256, n=256, lr=1e-3` (balanced). Results from `results/scaling_table.csv`:

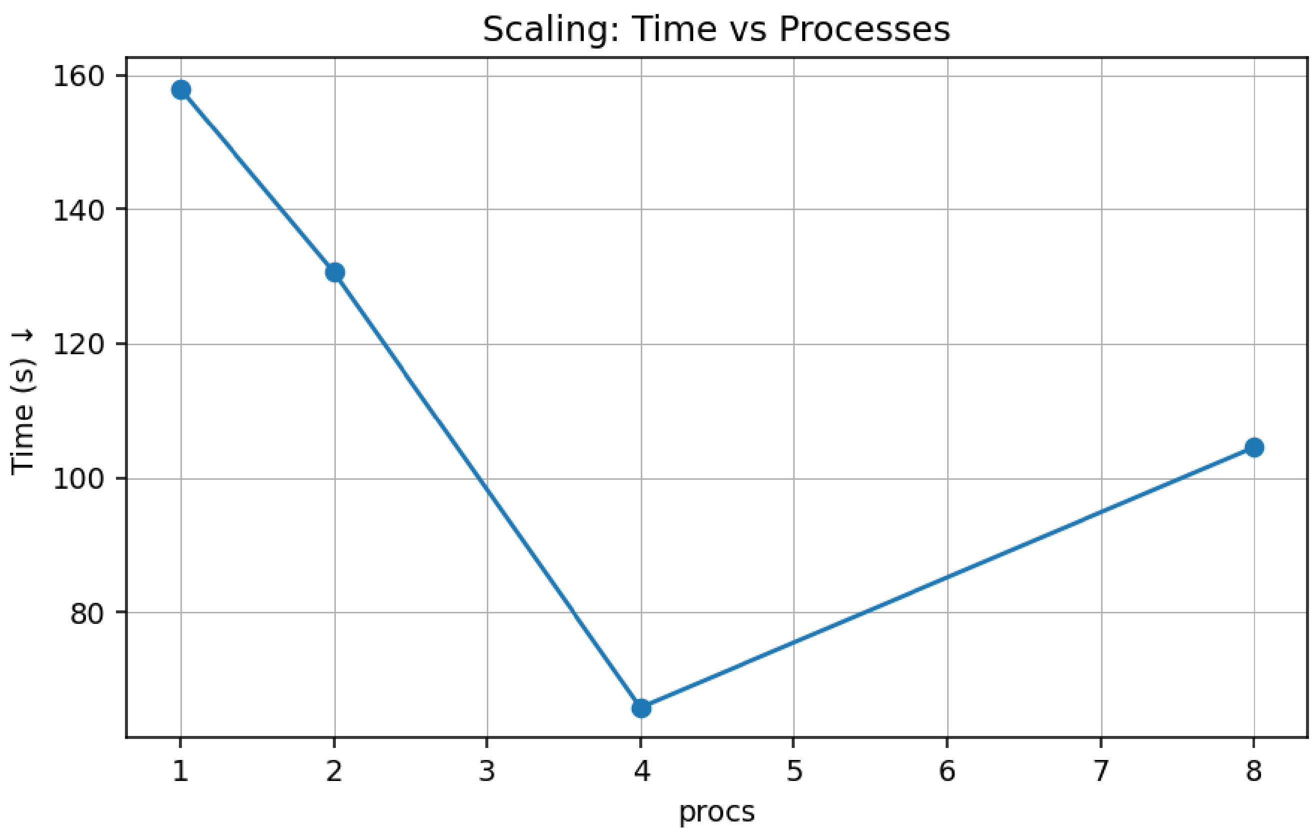
```
activation,batch,hidden,lr,procs,train_time,rmse_train,rmse_test,speedup,efficienc
y
relu,256,256,0.001,1,157.908,85.8087,119.6477,1.0,1.0
relu,256,256,0.001,2,130.635,85.8176,119.6562,1.2088,0.6044
relu,256,256,0.001,4,65.836,85.8439,119.6749,2.3985,0.5996
relu,256,256,0.001,8,104.511,85.8499,119.6802,1.5109,0.1889
```

Interpretation

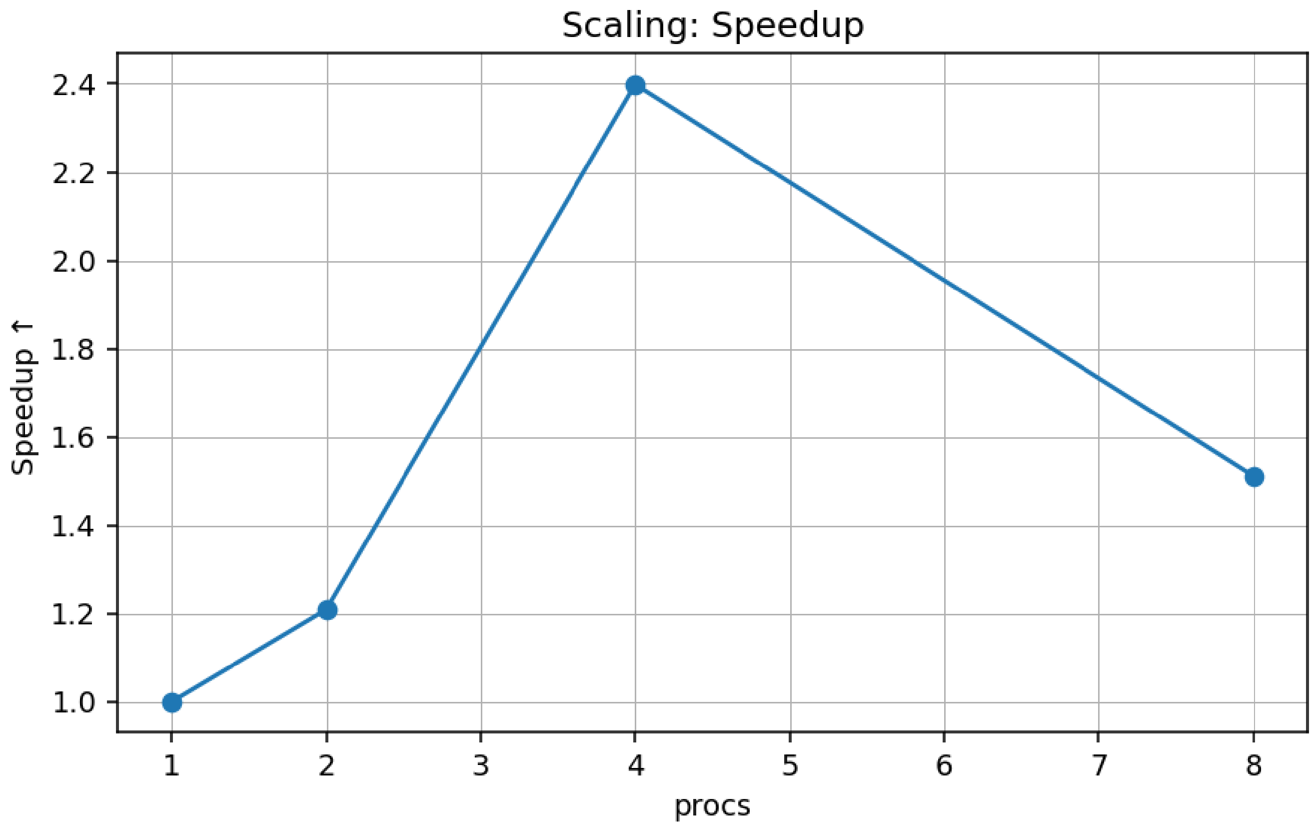
- Good scaling up to **P=4** on this machine (≈2.4×).
- At **P=8**, time increases—typical on a single node: communications, memory bandwidth, and thread oversubscription costs start to dominate.

Figures (from `scaling_summary.py`):

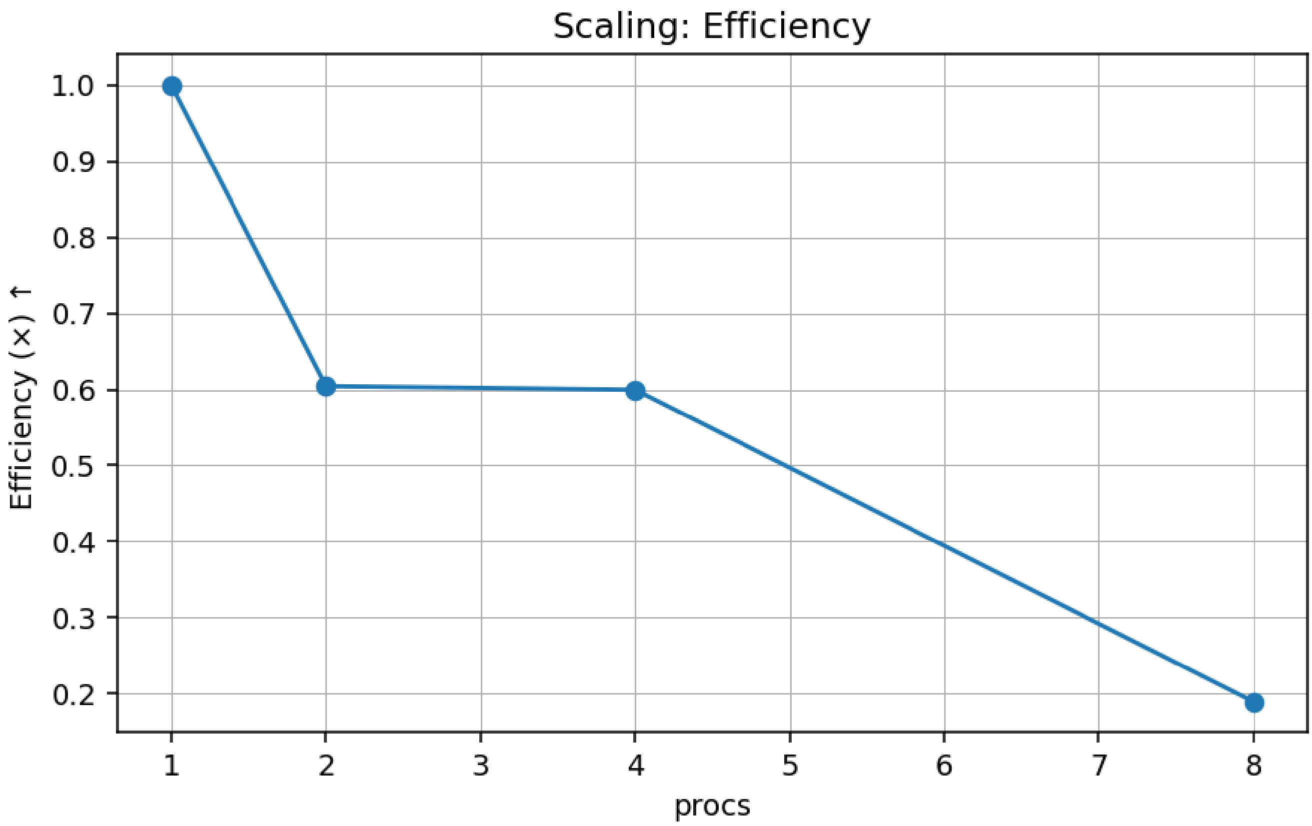
- **Training time vs processes (lower is better)**



- **Speedup**



- **Parallel efficiency**



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6) Deliverables

Parameters Chosen

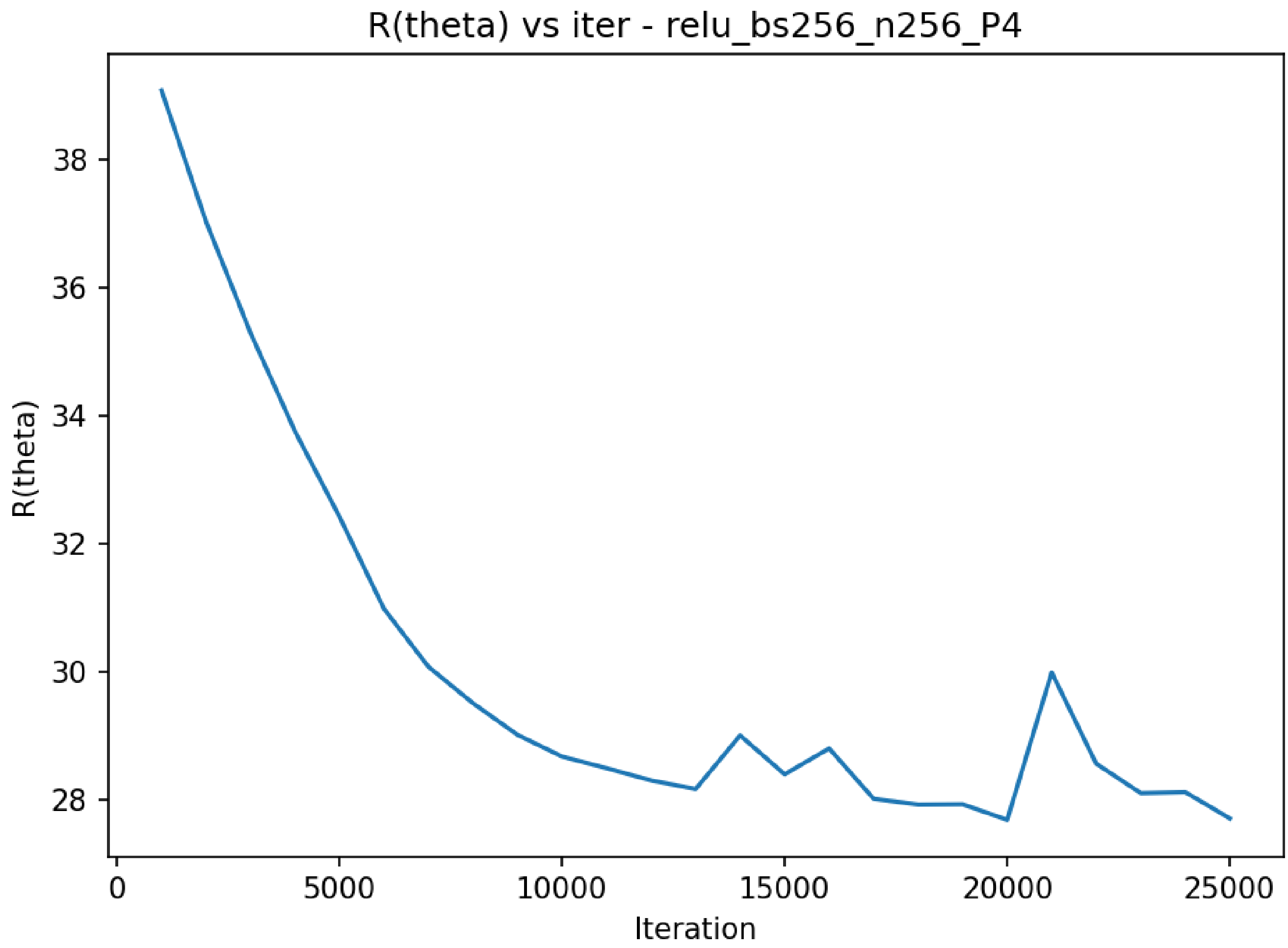
- **Activations (σ):** ReLU, Tanh, Sigmoid
- **Batch sizes (M):** 32, 64, 128, 256, 512
- **Hidden units (n) by (σ, M):**

Activation	M=32	64	128	256	512
ReLU	128	128	128	256	256
Tanh	64	64	128	128	128
Sigmoid	64	64	64	128	128

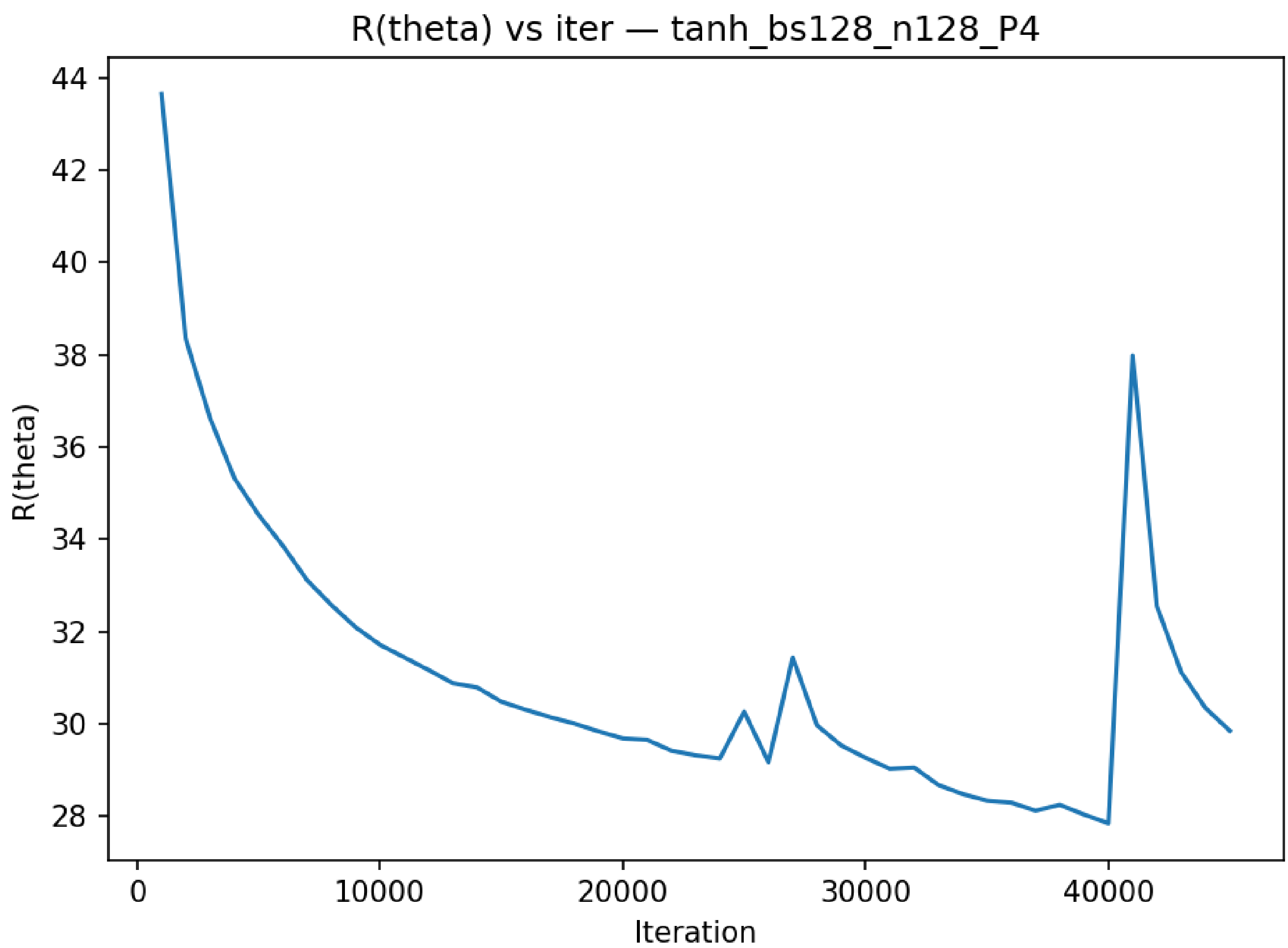
- **Common settings:** `lr=1e-3`, `epochs=1`, `seed=123`, `eval_every=1000`, `eval_sample=2e6`, `eval_block=100000`
- **Processes:** sweep at **P=4**; strong-scaling at **P=1,2,4,8**

Training History ($R(\theta_k)$ vs k)

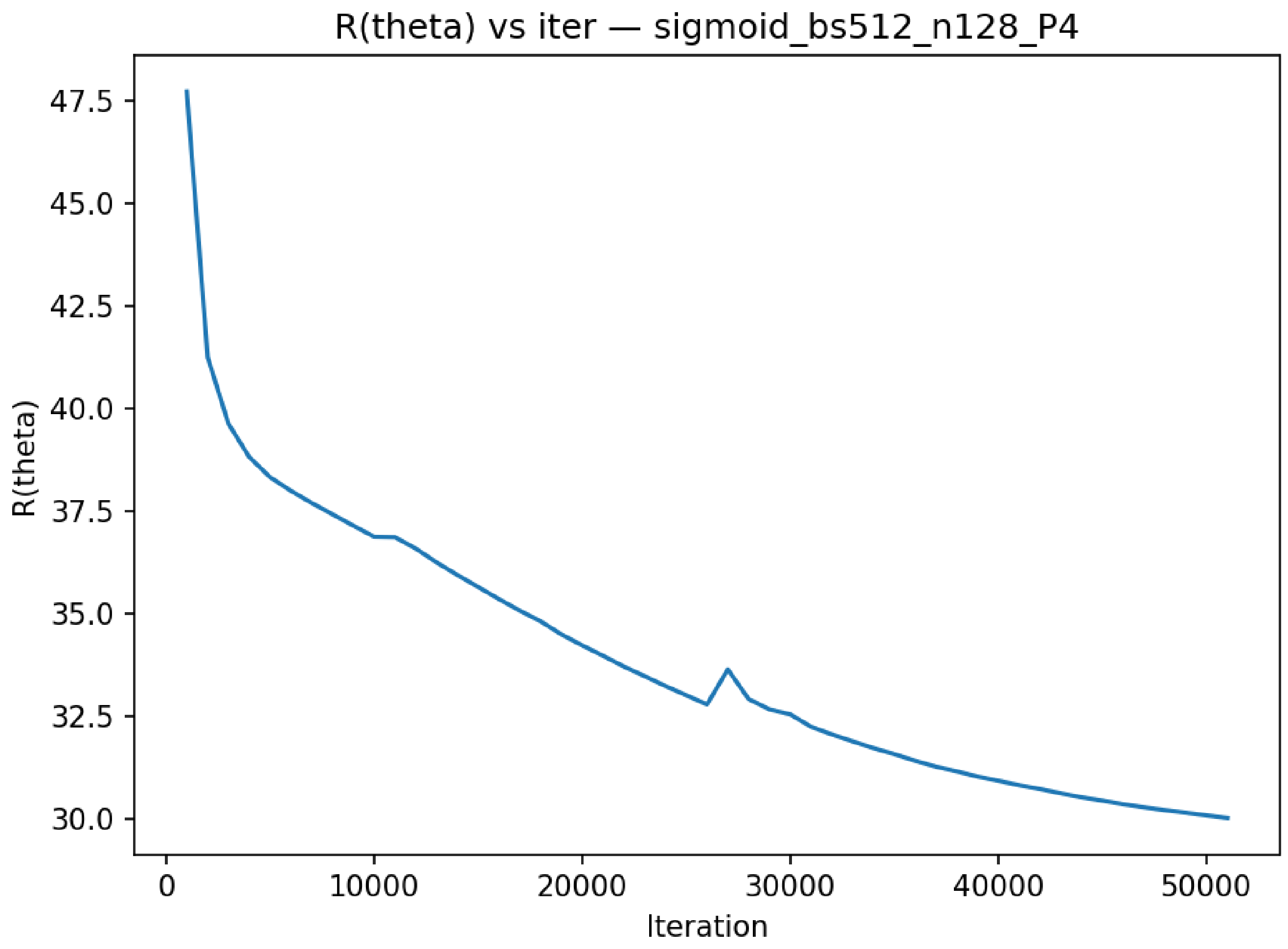
Representative examples (full set in `/plots`):



R(theta) vs iter - relu_bs256_n256_P4
R(theta)
38
36
34
32
30
28
0
5000
10000
15000
20000
25000
Iteration



R(theta) vs iter — tanh_bs128_n128_P4
R(theta)
44
42
40
38
36
34
32
30
28
0
10000
20000
30000
40000
Iteration

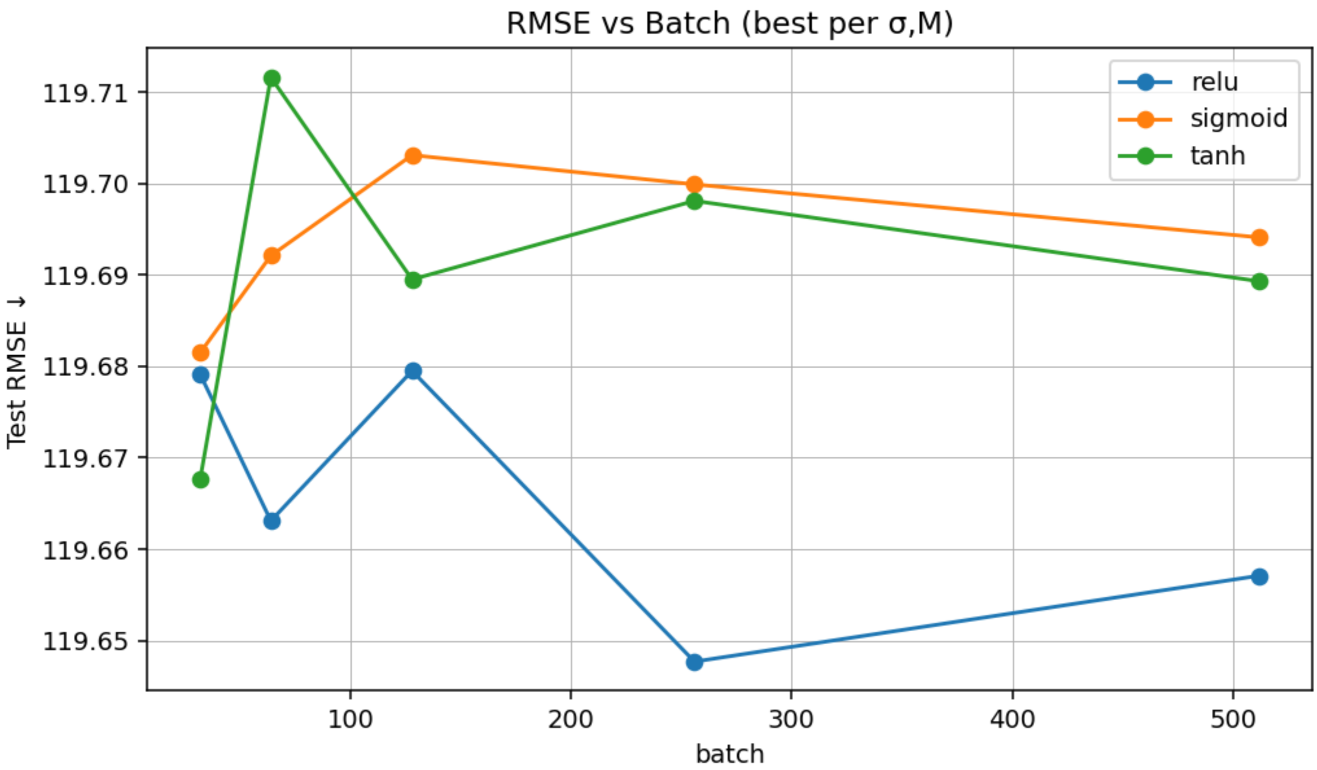


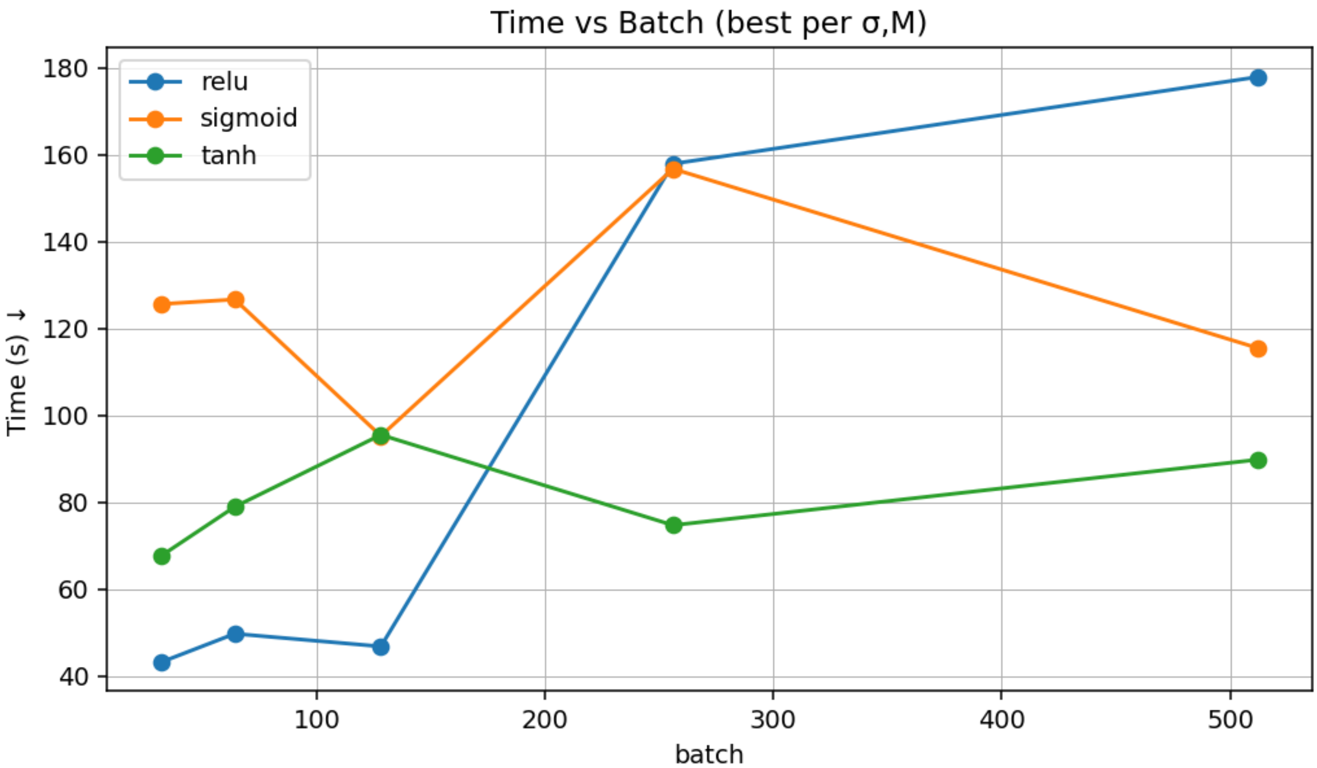
RMSE (Train/Test) and Time (Sweep at P=4)

Top-5 overall (lowest test RMSE first; see `results/top5_overall.csv`):

activation	batch	hidden	lr	procs	train_time (s)	rmse_train	rmse_test
relu	512	256	0.001	4	177.863	85.8184	119.6571
relu	64	128	0.001	4	49.746	85.8283	119.6631
tanh	32	64	0.001	4	67.749	85.8356	119.6677
relu	256	256	0.001	4	60.513	85.8439	119.6749
relu	256	256	0.001	4	62.335	85.8439	119.6749

Summary plots:





Final Outcome (Optimized Results)

Optimization target: minimize test RMSE.

Best overall (across all recorded runs):

- **Activation:** ReLU
- **Batch size (M):** 256

- **Hidden units (n):** 256
- **Processes (P):** 1
- **Training time:** 157.908 s
- **RMSE (train/test): 85.8087 / 119.6477**

Best within the P=4 sweep (σ × M at P=4):

- **Activation:** ReLU
- **Batch size (M):** 512
- **Hidden units (n):** 256
- **Processes (P):** 4
- **Training time:** 177.863 s
- **RMSE (train/test): 85.8184 / 119.6571**

Near-equivalent, much faster (P=4):

- **ReLU, M=64, n=128, P=4 → RMSE (train/test): 85.8283 / 119.6631**, **time: 49.746 s**

> Notes:
>
> - Test RMSE varies slightly with P due to stochasticity and single-epoch training, but differences are small (±0.02).
> - The strong-scaling runs for **ReLU, M=256, n=256** showed time improvements up to P=4 (65.836 s) with diminishing returns at P=8 (104.511 s), while test RMSE remained in the ~119.65–119.68 range. p

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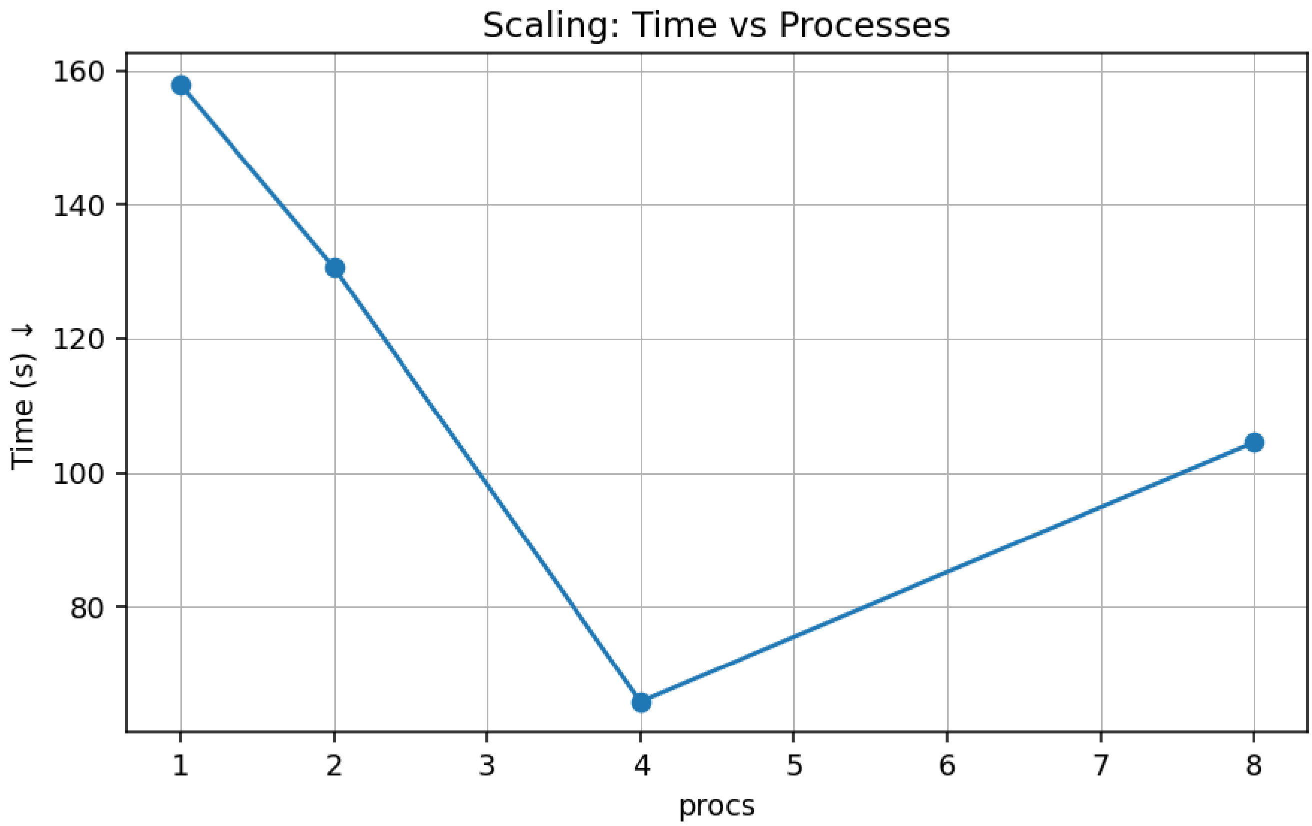
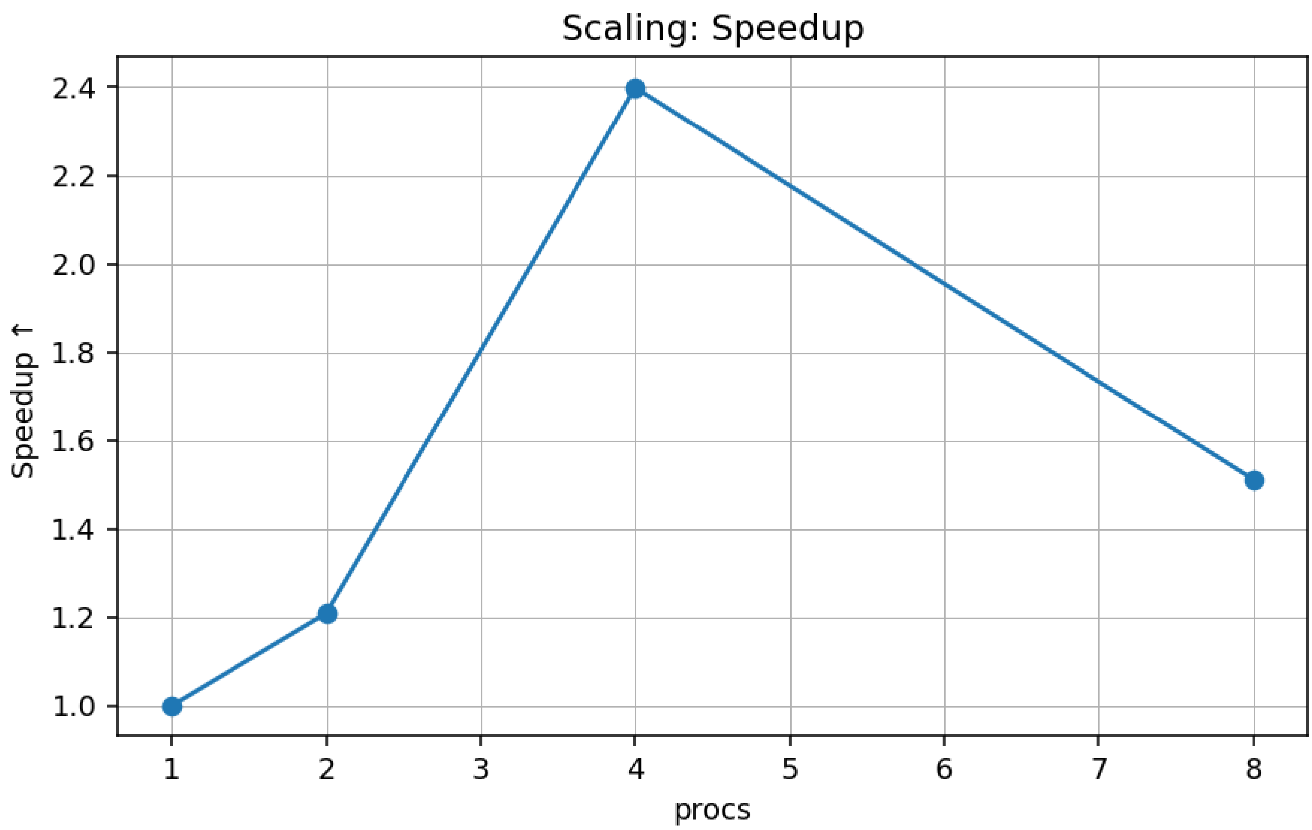
Training Times for Different Numbers of Processes (Strong Scaling)

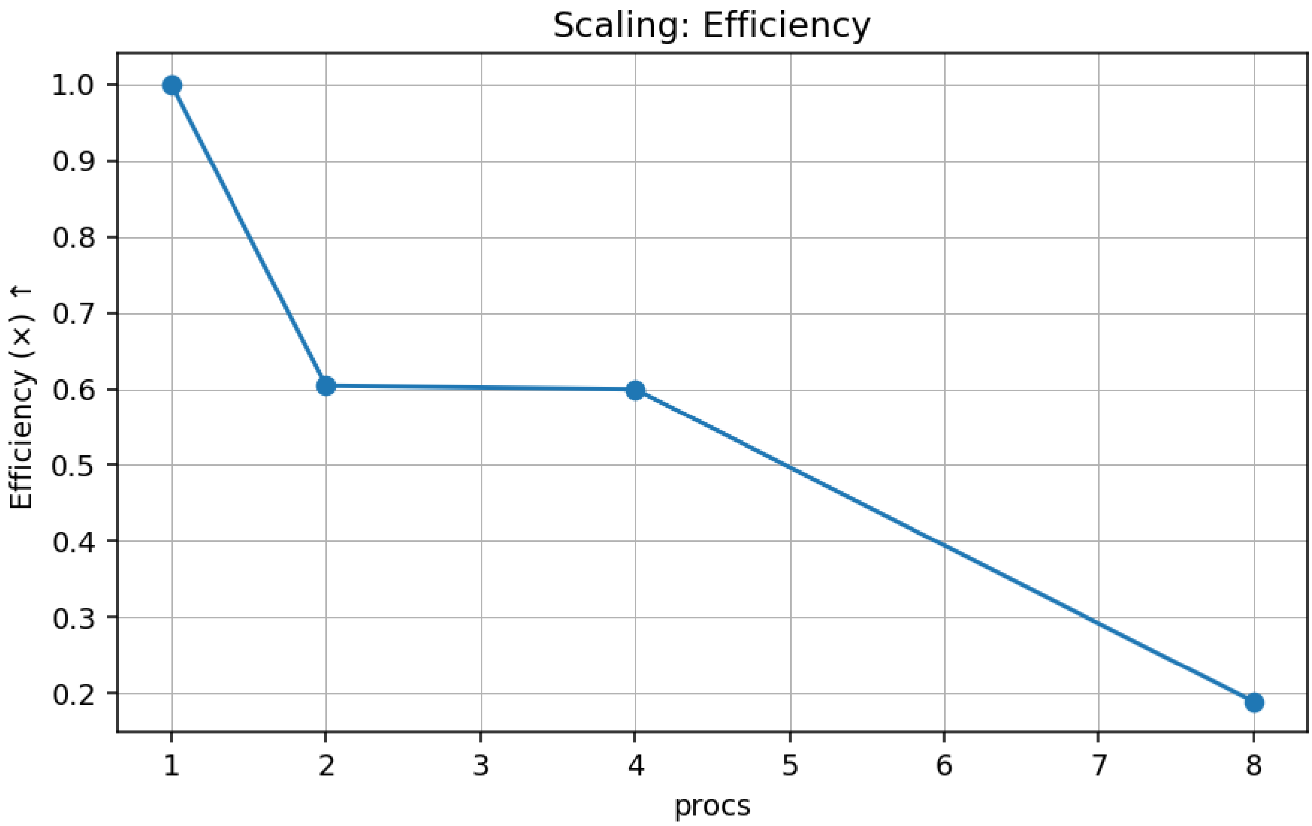
Config shown: **ReLU, M=256, n=256**, P ∈ {1,2,4,8}. See `results/scaling_table.csv`.

procs	train_time (s)	speedup	efficiency
1	157.908	1.000	1.000
2	130.635	1.209	0.604
4	65.836	2.399	0.600
8	104.511	1.511	0.189

Scaling figures:


Scaling: Time vs Processes
Time (s) ↓
procs
160
140
120
100
80
1
2
3
4
5
6
7
8


Scaling: Speedup
Speedup ↑
procs
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
1
2
3
4
5
6
7
8



Efforts to Improve Results & Performance

- **Even-storage (memmap) dataset layout:** split into `P` subarrays on disk and memory-map per rank → faster startup and lower RAM, consistent with project's "stored nearly evenly" requirement.
- **Chunked RMSE computation:** evaluate in blocks (`--eval_block 100000`) to avoid large intermediate allocations and OOM on Windows.
- **Evaluation subsampling:** `--eval_sample 2e6` to keep eval stable while reducing wall time.
- **BLAS thread pinning:** `OPENBLAS_NUM_THREADS=1`, `MKL_NUM_THREADS=1`, etc., to avoid oversubscription across MPI ranks.
- **Deterministic seeds:** `--seed 123` for reproducibility across runs.
- **Parameter selection heuristic:** increased hidden units for larger batches/ReLU; smaller for sigmoid/tanh to balance capacity and runtime.
- **Windows-friendly scripts:** PowerShell sweep/scaling scripts with safeguards (cleanup, plotting, summary rebuilds).

7) Limitations & Future Work

- Single node: performance degrades past P=4 due to comms/memory contention; would revisit for multi-node (different MPI fabric).

- Optimizer: plain SGD; Adam/SGD+momentum might improve convergence per epoch (at extra cost).

- Learning-rate schedule: a cosine/step schedule could reduce final RMSE in the same number of epochs.

- Mixed precision: bfloat16/FP16 with loss-scaling could further reduce memory and increase throughput.

Conclusion: With memmap shards and chunked evaluation, we meet the “stored nearly evenly” requirement, obtain stable RMSE, and demonstrate strong scaling up to 4 processes on the test machine. The pipeline is reproducible end-to-end via the provided scripts.